

Temperature Dependence of Thermal Expansivity of Carbon Fullerene and 20-nm Nickel Nanocrystal

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ABSTRACT

In the present study, the authors have determined the thermoelastic properties such as volume thermal expansion coefficient, volume expansion and bulk modulus for fullerene(C_{60}) and 20-nm nickel nanocrystal using a simple method as suggested by Zheng-Hua Fang [Solid state Sciences,10 (2008), 950]. The calculated values of thermal expansivity and volume thermal expansion are compared to the available data based on molecular simulation method and the results of thermal expansivity obtained for 20-nm nickel are compared to the available experimental data. A good agreement has been obtained between the theoretically calculated results and available experimental data.

Keywords: Thermal expansivity, thermal expansion coefficient, equation of state, nanocrystals.

1. INTRODUCTION

In recent years, there has been intensive activity, both experimental and theoretical, in exploring fascinating physical properties of fullerenes and nanocrystalline materials. The study of nanocrystalline materials with dimensions less than 100 nm in an active area of research in physics, chemistry and engineering as they provide vital information on their intrinsic microstructure characteristics^{1,2}. Nano-crystals have large

surface to volume ratio, and surface effects take on a significance that is normally inconsequential for bulk materials. One of the main areas of scientific interest of nanocrystalline materials is their thermodynamic properties because their stability and their atomic interactions are related in complex ways to their mechanical properties. Therefore, it is of great fundamental interest to explore thermodynamic consequences of a material system with interfacial regions.

The basic C_{60} structure consists of 60 carbon atoms that link together to form a hollow cage-like structure. The structure consists of 32 faces of which 20 are hexagons and 12 are pentagons. Of these no two pentagons share a common side. Several physical properties such as compressibility, bulk modulus and Debye temperature have been studied for bulk fullerenes C_{60} ^{3,4} but less literature is available for a single fullerene (C_{60}). The Nanocrystalline nickel (n-Ni), an important nanocrystalline metal, has been also the subject of considerable experimental and theoretical work during past years^{5,6}. The mechanical^{7,8}, electrical behavior⁹, diffusion coefficient and vibrational modes^{10,11} of n-Ni has been widely investigated. Nickel is a transition ferromagnetic 3d metal that is widely used as catalyst at extreme conditions¹².

Recently Haijun Shen¹³ made an attempt to calculate the compressive mechanical properties of C_{60} by using the Tersoff-type potential based on molecular dynamic simulations. In the present study, we have determined the thermo elastic properties such as thermal expansivity, thermal expansion coefficient, volume expansion and bulk modulus for fullerene (C_{60}) and 20-nm nickel nanocrystal using a simple method as suggested by Zheng-Hua Fang [14]. He has developed a method based on approximation, as suggested by Wang *et al* [15], that the temperature derivative of the work done by thermal pressure approaches a constant at high temperature. Assuming this fact, Zheng-Hua Fang¹⁴ has recently reported the theoretically calculated results of elastic moduli and thermal expansivity of MgO and CaO minerals which are found in good agreement with

their corresponding experimental data. To test the validity and applicability of this model theory in nanomaterials, we have considered single fullerene (C_{60}) and 20-nm nickel nanocrystal in the present investigation because the experimental data are readily available on them. The method of analysis is described in section 2 and the results achieved in the present study are discussed and compared with corresponding experimental data in section 3.

2. METHOD OF ANALYSIS

A theory based on the critical behavior of vibrational elongation¹⁶ is defined as the effective increase in the interatomic distance due to the lattice vibrations. The anharmonicity of the lattice plays an important role in the concept of vibrational elongation produced in crystal. The equation of state for the analysis of thermal expansion coefficient can be derived in terms of only the variable parameter temperature. Many theoretical studies suggest that the product αK_T is insensitive to volume over a range of temperatures. However, Singh *et al.*¹⁷ have recently showed that the product αK_T does not remain constant within the accuracy of experiment but decreases with temperature above the Debye temperature, and the product αK_TV changes evidently less with temperature as compared to the product αK_T . Since the nanomaterials are much harder in comparison to their counterpart bulk materials, the product $\alpha_T K_TV$ can be assumed to be constant above the Debye temperature.

Assuming that under the effect of temperature the product of thermal

expansion coefficient (α), volume (V) and isothermal bulk modulus (K_T) remains constant, we can write

$$K_T V = \alpha_o K_o V_o \quad (1)$$

The isothermal Anderson - Gruneisen parameter δ_T is written as follows:

$$\delta_T = -\frac{1}{\alpha_T K_T} \left(\frac{\partial K_T}{\partial T} \right)_P, \quad (2)$$

The thermal expansivity is defined as

$$\alpha_T = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P, \quad (3)$$

Using the definition of thermal expansivity in equation (2), we get

$$\delta_T = -\frac{V}{K_T} \left(\frac{\partial K_T}{\partial V} \right)_P \quad (4)$$

The isothermal Anderson-Gruneisen parameter δ_T can also be defined as follows¹⁸:

$$\delta_T = \delta_o \frac{V}{V_o} \quad (5)$$

Where δ_o and V_o are respectively, the Anderson-Gruneisen parameter δ_T and the volume V both at room temperature and zero pressure.

Substituting equations (5) and (1) in equation (2), we get

$$\left(\frac{\partial K_T}{\partial V} \right)_P = \alpha_o K_o \delta_o \quad (6)$$

Integrating eq. (6) over temperature at $P=0$, we get the following expression of

isothermal bulk modulus K_T as the function of temperature, viz,

$$K_T = K_o [1 - \alpha_o \delta_o (T - T_o)] \quad (7)$$

Similarly, the following expression for the temperature dependence of volume thermal expansion of nanomaterials can be obtained by substituting equations (2) and (7) into equation (1) and integrating it over temperature, i.e.

$$\frac{V}{V_o} = 1 - \frac{1}{\delta_o} \ln[1 - \alpha_o \delta_o (T - T_o)] \quad (8)$$

The variation of thermal expansion coefficient of nanomaterials with temperature is simply found by using equation (8) in equation (1), i.e.

$$\frac{\alpha_T}{\alpha_o} = \frac{V_o}{V} [1 - \alpha_o \delta_o (T - T_o)]^{-1} \quad (9)$$

The equations (7-9) obtained in the present work are thus the simplest forms of equations of state which can be used straightforward to calculate the bulk modulus and thermal expansion properties of nanocrystals.

3. RESULTS AND DISCUSSION

In the present study, we have calculated the temperature dependence of relative bulk modulus (K_T / K_o), volume thermal expansion ($\frac{V}{V_o}$) and thermal expansion coefficient ($\frac{\alpha_T}{\alpha_o}$) of carbon fullerene (C_{60}) and 20-nm nickel nanocrystal, using equations (7), (8), (9) respectively at different temperatures. The equations (7-9) are entirely free from crystal potential and need only initial values of

input parameters such as Anderson-Gruneisen parameter (δ_o), volume thermal expansion coefficient (α_o) at zero pressure and room temperature T_o . The calculated values are plotted with temperature and compared to the available experimental data^{19,21} for the sake of comparison. Graphically the results are shown in figures 1-3 for fullerene and figures 4-6 for nickel nanocrystal. It is noted that our calculated values are in good agreement to the available experimental data for these materials. The input parameters¹⁹⁻²² used for calculation work are given in table 1.

The present results confirm that the equations of state⁷⁻⁹ predict the temperature dependence of thermo elastic properties of

nanomaterials satisfactorily. It may thus be emphasized here that the equations of state described in the present paper explain the thermal properties not only for bulk materials¹⁴ but also for nanomaterials with the same potential. The success of these equations can be traced from thermal behavior of bulk material as available in the literature¹⁴ and nanomaterials as depicted in the present study.

Table 1: Input data used in the present study at room temperature T_o

Nanomaterials	$\alpha_o(10^{-6}K^{-1})$	δ_o	$K_o(GPa)$
C ₆₀	17.27 [19]	122	491[20]
20-nm Ni	33.0 [21]	26.34	228[22]

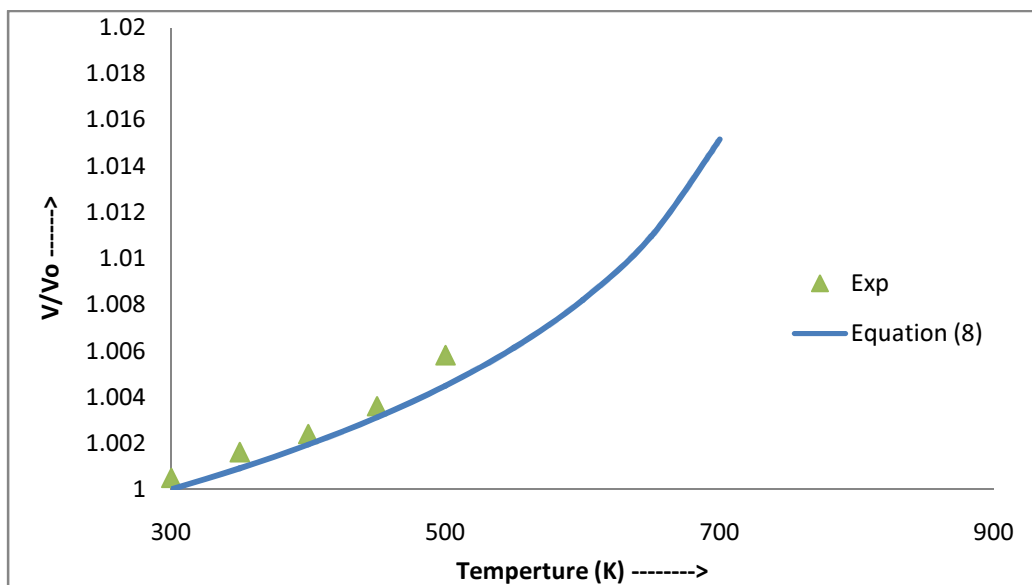


Figure1: Shows the variation of Volume thermal expansion ($\frac{V}{V_o}$) of Carbon fullerene (C₆₀) at different temperatures T (kelvin)

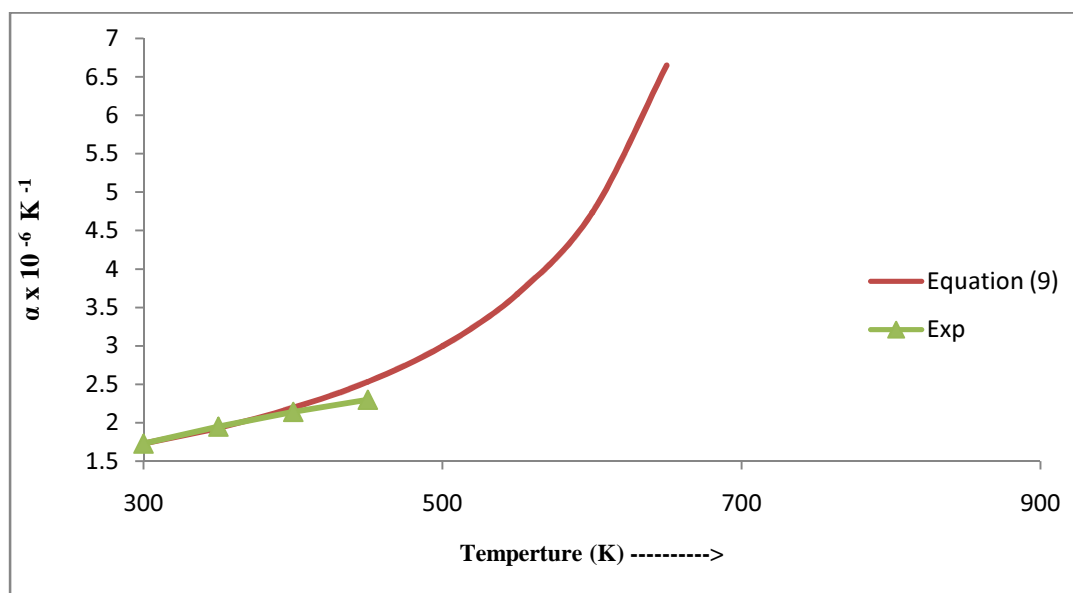


Figure 2: Shows the variation of Thermal expansivity α of Carbon fullerene (C_{60}) at different temperatures T (kelvin)

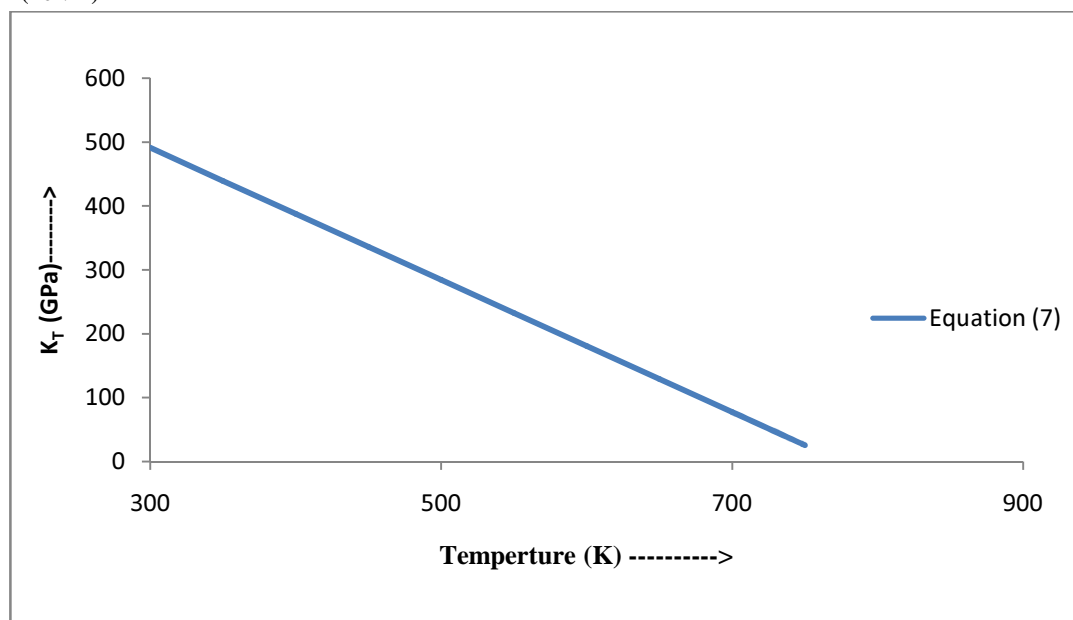


Figure 3: Shows the variation of bulk modulus K_T (GPa) of Carbon fullerene (C_{60}) at different temperatures T (kelvin)

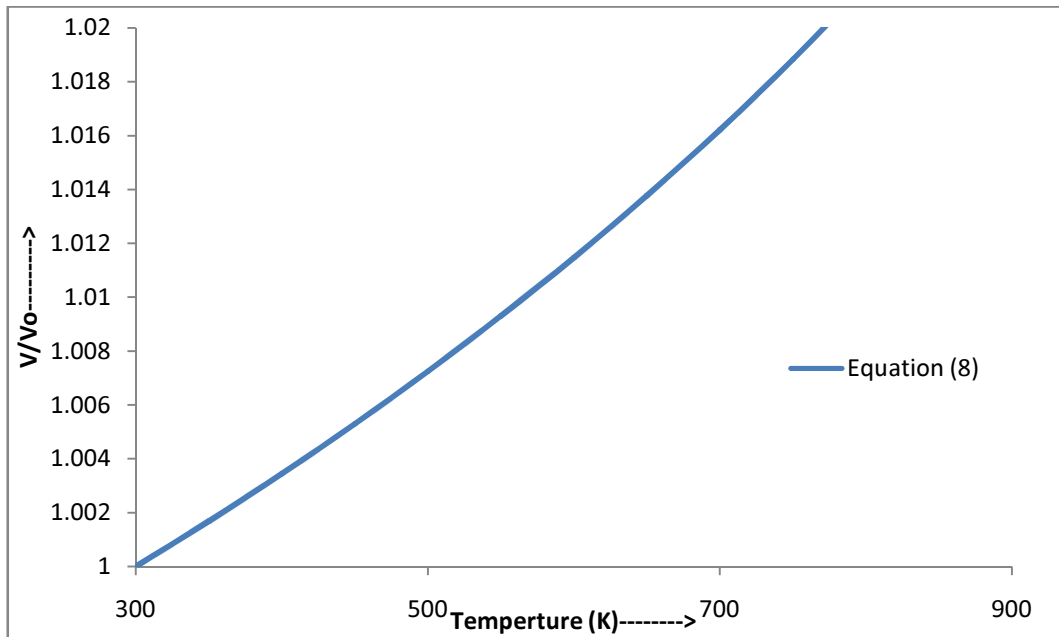


Figure 4: Shows the variation of Volume thermal expansion ($\frac{V}{V_o}$) of 20 nm-Ni at different temperatures T (kelvin)

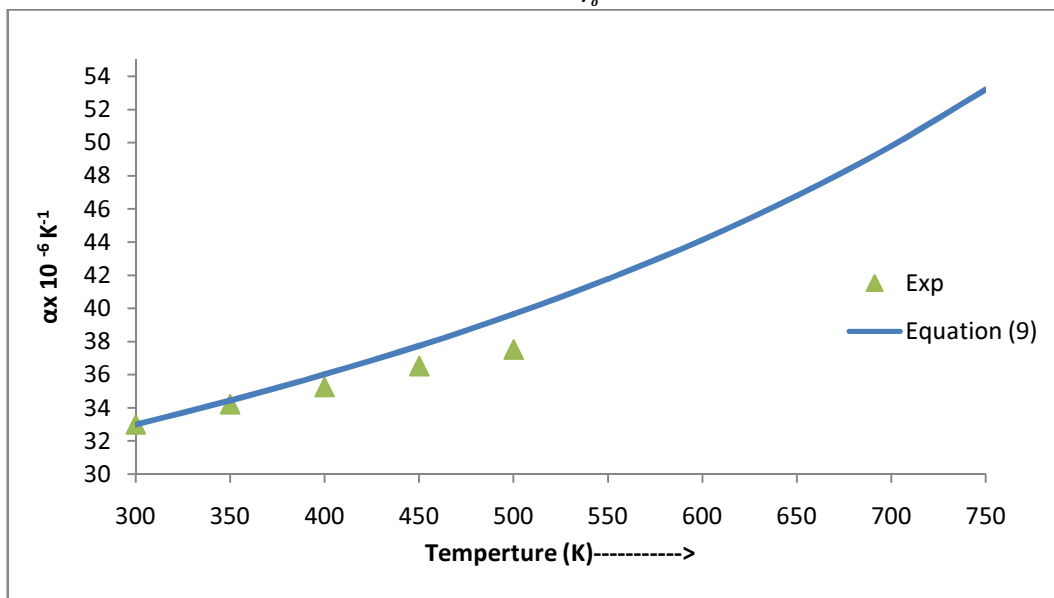


Figure5: Variation of Thermal expansivity α of 20nm Ni at different temperatures T (kelvin)

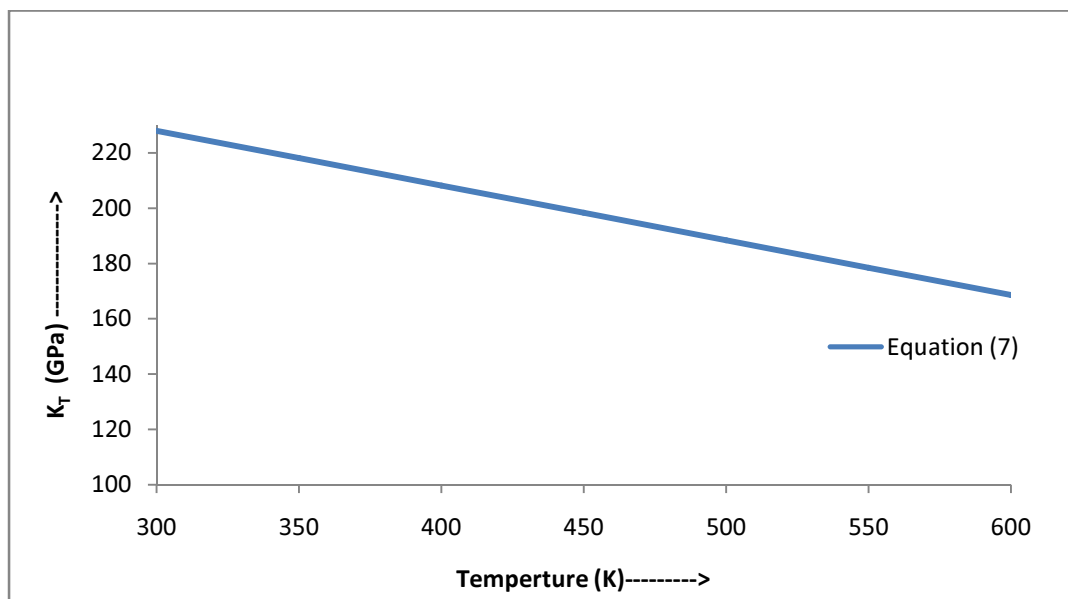


Figure 6: Variation of bulk modulus K_T (GPa) of 20 nm-Ni at different temperatures T (kelvin)

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